A Systematic Methodology for Design of Emulsion Based Chemical Products

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A Systematic Methodology for Design of Emulsion Based Chemical Products

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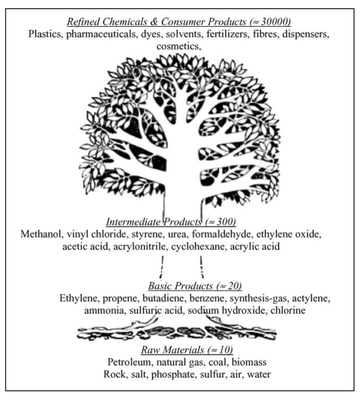
1. CHEMICAL PRODUCT DESIGN AND EMULSIONS

- Chemical product design aims to find a product exhibiting a set of deisrable or specified behavior
- Chemical industry is shifting from commodities towards higher value added products
- Higher value added products gain their value from a molecular or micro-structure
- Emulsions are largely used as commercial products: food, cosmetic, household and health-care industries
- Surfactant and emulsion properties may require dedicated models



2. A SYSTEMATIC METHODOLOGY

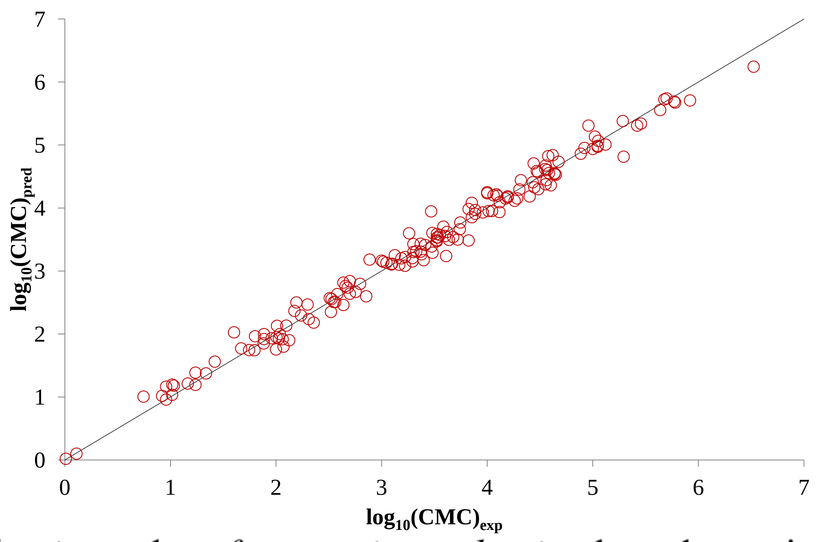
Step	Input	Performed Action	Output
Step 1	Information about the product	Understanding of needs, translation into target properties in terms of constraints to match	List of main needs, secondary needs and target properties with boundaries
Step 2	List of main needs	Find chemicals suitable as active ingredient(s), select the most advantageous and search/calculate main properties	Candidate active ingredient with its main properties
Step 3	Candidate active ingredient with its main properties	Find chemicals suitable as dispersed phase solvents, select the most advantageous and search/calculate main properties	Candidate dispersed phase solvent with its main properties
Step 4	Candidate active ingredient and dispersed phase solvent with their main properties	Find chemicals suitable as continuous phase solvents, select the most advantageous and search/calculate main properties	Candidate continuous phase solvent with its main properties
Step 5	Candidate active ingredient dispersed and continuous phase solvents with their main properties	Find chemicals suitable as emulsifiers, select the most advantageous and search/calculate main properties	Candidate emulsifier with its main properties
Step 6	List of secondary needs, candidate dispersed and continuous phase solvents with their main properties	Find chemicals suitable as additives, select the most advantageous and search/calculate main properties	Candidate additives with their main properties
Step 7	List of constraints on target properties, all ingredients	Find overall composition of selected ingredients	Product to be experimentally verified (Stage-2)

3. SELECTION CRITERIA

- *Constraints*
  - Low toxicity → Lethal concentration: $LC_{50} > 3{,}16$
  - Safety → Flash point: FP > 60°C
  - Legislation → Some chemicals are not allowed
  - Critical temperatures → Melting point, boiling point, peculiar critical temperatures of surfactants
  - Stability → Surfactant above critical micelle concentration
- *Selection criteria*
  - Optimize the effectiveness (it differs ingredient by ingredient and it is estimated mainly with knowledge base)
  - Minimize the cost

4. SURFACTANT PROPERTY MODELING

- *Critical micelle concentration* (158 data)
  - Non-ionic surfactants, T = 25°C
  - M&G GC⁺ method: $f(X) = \sum_i N_i C_i + w \sum_j M_j D_j + z \sum_k O_k E_k$
  - $R^2 = 0{,}99$



- *Cloud point* and *surface tension reduction* have been similarly modeled with high fitting quality
- Modeling of *ionic surfactant* properties will be the next step

5. A CONCEPTUAL CASE STUDY

- UV sunscreen, emulsified form
- Proposed formulation to be experimentally validated

Avobenzone	0,99%		
Octyl Salycilate	1,22%	Octyl Esaethylene Oxide	0,09%
Zinc Oxide	8,56%	α-Tocopherol	0,34%
Butyl Acetate	32,4%	Heptylparaben	0,59%
Water	54,9%	*laevo*-Menthol	0,91%

6. CONCLUSIONS

- A systematic methodology for design of emulsion-based products has been developed
- Its application has been illustrated through the conceptual case study of an emulsified UV sunscreen
- The development of dedicated models for pure compound (surfactant) as well as mixture (emulsion) properties is fundamental
- A second stage, model-experiment based further refinement and/or validation has been considered and needs to be developed
- The work-flow will be implemented into a software to allow virtual product design

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